

Biocatalysis

Burlington House,
London, United Kingdom
and online

22 – 24 May 2024



FARADAY DISCUSSIONS

Volume 252, 2024

The Faraday Community for Physical Chemistry of the Royal Society of Chemistry, previously the Faraday Society, was founded in 1903 to promote the study of sciences lying between chemistry, physics and biology.

Editorial Staff

Executive Editor

Michael A. Rowan

Deputy Editor

Vikki Pritchard

Development Editors

Bee Hockin, Andrea Carolina Ojeda Porras

Editorial Manager

Gisela Scott

Associate Editorial Manager

Robin Brabham

Publishing Editors

Robert Hinde and Samuel Oldknow

Editorial Assistant

Daphne Houston

Publishing Assistants

David Bishop and Lee Colwill

Publisher

Jeanne Andres

Faraday Discussions (Print ISSN 1359-6640, Electronic ISSN 1364-5498) is published 8 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WE.

Volume 252 ISBN 978-1-83767-387-2

2024 annual subscription price: print+electronic £1272

US \$2240; electronic only £1212, US \$2133.

Customers in Canada will be subject to a surcharge to cover GST.

Customers in the EU subscribing to the electronic version only will be charged VAT.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WE, UK
Tel +44 (0)1223 432398; E-mail orders@rsc.org

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Printed in the UK



Faraday Discussions

Faraday Discussions are unique international discussion meetings that focus on rapidly developing areas of chemistry and its interfaces with other scientific disciplines.

Scientific Committee volume 252

Co-Chairs

Adrian Mulholland, University of Bristol, UK
Nicholas Turner, University of Manchester, UK

Committee

Meilan Huang, Queens University Belfast, UK
Amanda Jarvis, University of Edinburgh, UK

Faraday Standing Committee on Conferences

Chair

Susan Perkin, University of Oxford, UK

David Fermin, University of Bristol, UK

Secretary

Susan Weatherby, Royal Society of Chemistry, UK

Dwayne Heard, University of Leeds, UK

David Lennox, University of Glasgow, UK

George Booth, King's College London, UK

Angelos Michaelides, University College London, UK

Rachel Evans, University of Cambridge, UK

Julia Weinstein, University of Sheffield, UK

Advisory Board

Vic Arcus, The University of Waikato, New Zealand

Michel Orrit, Leiden University, The Netherlands

Timothy Easun, Cardiff University, UK

Zhong-Qun Tian, Xiamen University, China

Dirk Guldí, University of Erlangen-Nuremberg, Germany

Siva Umaphathy, Indian Institute of Science, Bangalore, India

Marina Kuimova, Imperial College London, UK

Bert Weckhuysen, Utrecht University, The Netherlands

Luis Liz-Marzán, CIC biomaGUNE, Spain

Julia Weinstein, University of Sheffield, UK

Andrew Mount, University of Edinburgh, UK

Sihai Yang, University of Manchester, UK

Frank Neese, Max Planck Institute for Chemical Energy Conversion, Germany

Information for Authors

This journal is © the Royal Society of Chemistry 2024. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

© The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

Registered charity number: 207890



Biocatalysis

Faraday Discussions

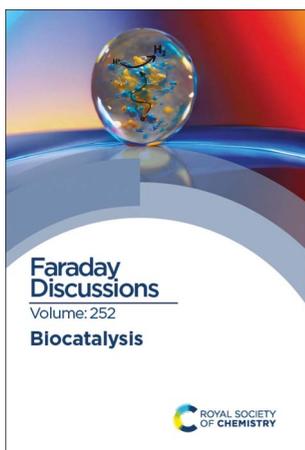
www.rsc.org/faraday_d

A General Discussion on Biocatalysis was held in London, UK and online on the 22nd, 23rd and 24th of May 2024.

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

CONTENTS

ISSN 1359-6640; ISBN 978-1-83767-387-2



Cover

See Valetti *et al.*, *Faraday Discuss.*, 2024, **252**, 223–240.

[FeFe] hydrogenase with intrinsic protection from oxidative damage can shed light on simple yet efficient catalysis on protons and electrons.

Image reproduced with permission of Francesca Valetti from Francesca Valetti *et al.*, *Faraday Discuss.*, 2024, **252**, 223–240.

INTRODUCTORY LECTURE

- 9 Spiers Memorial Lecture: Engineering biocatalysts**
Donald Hilvert

PAPERS AND DISCUSSIONS

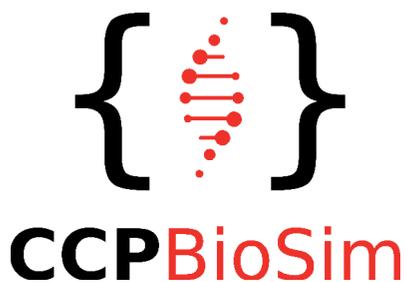
- 29 Indigo production identifies hotspots in cytochrome P450 BM3 for diversifying aromatic hydroxylation**
Douglas J. Fansher, Jonathan N. Besna and Joelle N. Pelletier
- 52 Tuning the peroxidase activity of artificial P450 peroxygenase by engineering redox-sensitive residues**
Fengjie Jiang, Zihan Wang and Zhiqi Cong
- 69 Exploring the selectivity of cytochrome P450 for enhanced novel anticancer agent synthesis**
Janko Čivič, Neil R. McFarlane, Joleen Masschelein and Jeremy N. Harvey



EXHIBITOR: AMANO ENZYME



SPONSOR: CCPBIOSIM



POSTER SPONSORSHIP: CATALYSIS SCIENCE AND TECHNOLOGY





- 89 On synergy between ultrahigh throughput screening and machine learning in biocatalyst engineering**
Maximilian Gantz, Simon V. Mathis, Friederike E. H. Nintzel, Pietro Lio and Florian Hollfelder
- 115 High-throughput selection of (new) enzymes: phage display-mediated isolation of alkyl halide hydrolases from a library of active-site mutated epoxide hydrolases**
Marija Blazic, Candice Gautier, Thomas Norberg and Mikael Widersten
- 127 Enzyme evolution, engineering and design: mechanism and dynamics: general discussion**
- 157 Enhancement of essential cofactors for *in vivo* biocatalysis**
Pattarawan Intasian, Chalermroj Sutthaphirom, Oliver Bodeit, Duangthip Trisrivirat, Ninlapan Kimprasoot, Juthamas Jaroensuk, Barbara Bakker, Edda Klipp and Pimchai Chaiyen
- 174 Developing deprotectase biocatalysts for synthesis**
Lisa Kennedy, Mariyah Sajjad, Michael A. Herrera, Peter Szieber, Natasza Rybacka, Yinan Zhao, Craig Steven, Zainab Alghamdi, Ivan Zlatkov, Julie Hagen, Chloe Lauder, Natalie Rudolfova, Magdalena Abramiuk, Karolina Bolimowska, Daniel Joynt, Angelica Lucero, Gustavo Perez Ortiz, Annamaria Lilienkampff, Alison N. Hulme and Dominic J. Campopiano
- 188 Retuning the potential of the electrochemical leaf**
Marta M. Dolińska, Adam J. Kirwan and Clare F. Megarity
- 208 Surveying the scope of aromatic decarboxylations catalyzed by prenylated-flavin dependent enzymes**
Anushree Mondal, Pronay Roy, Jaclyn Carrannanto, Prathamesh M. Datar, Daniel J. DiRocco, Katherine Hunter and E. Neil G. Marsh
- 223 Oxygen-resistant [FeFe]hydrogenases: new biocatalysis tools for clean energy and cascade reactions**
Francesca Valetti, Simone Morra, Lisa Barbieri, Sabrina Dezzani, Alessandro Ratto, Gianluca Catucci, Sheila J. Sadeghi and Gianfranco Gilardi
- 241 Biocatalytic pathways, cascades, cells and systems: general discussion**
- 262 Computation-guided engineering of distal mutations in an artificial enzyme**
Fabrizio Casilli, Miquel Canyelles-Niño, Gerard Roelfes and Lur Alonso-Cotchico
- 279 Designing Michaelases: exploration of novel protein scaffolds for iminium biocatalysis**
Alejandro Gran-Scheuch, Stefanie Hanreich, Iris Keizer, Jaap W. Harteveld, Eelco Ruijter and Ivana Drienovská
- 295 An efficient pyrrolysyl-tRNA synthetase for economical production of MeHis-containing enzymes**
Amy E. Hutton, Jake Foster, James E. J. Sanders, Christopher J. Taylor, Stefan A. Hoffmann, Yizhi Cai, Sarah L. Lovelock and Anthony P. Green
- 306 Harnessing conformational dynamics in enzyme catalysis to achieve nature-like catalytic efficiencies: the shortest path map tool for computational enzyme redesign**
Cristina Duran, Guillem Casadevall and Silvia Osuna

- 323 **Computational study of the mechanism of a polyurethane esterase A (PueA) from *Pseudomonas chlororaphis***
Katarzyna Świderek, Sergio Martí, Kemal Arafet and Vicent Moliner
- 341 **Friends and relatives: insight into conformational regulation from orthologues and evolutionary lineages using KIF and KIN**
Daria Yehorova, Rory M. Crean, Peter M. Kasson and Shina Caroline Lynn Kamerlin
- 354 **Artificial, biomimetic and hybrid enzymes: general discussion**
- 387 **Degradation of PET microplastic particles to monomers in human serum by PETase**
Ximena Lopez-Lorenzo, David Huetting, Elliott Bosshard and Per-Olof Syrén
- 403 **Towards controlling activity of a peptide asparaginyl ligase (PAL) by lumazine synthetase compartmentalization**
T. M. Simon Tang and Louis Y. P. Luk
- 422 **On the biocatalytic synthesis of silicone polymers**
Yuqing Lu and Lu Shin Wong
- 431 **An engineered T7 RNA polymerase for efficient co-transcriptional capping with reduced dsRNA byproducts in mRNA synthesis**
Mathew Miller, Oscar Alvizo, Scott Baskerville, Avinash Chintala, Chinping Chng, Justin Dassie, Jonathan Dorigatti, Gjalt Huisman, Stephan Jenne, Supriya Kadam, Neil Leatherbury, Stefan Lutz, Melissa Mayo, Arpan Mukherjee, Antoinette Sero, Stuart Sundseth, Jonathan Penfield, James Riggins and Xiyun Zhang
- 450 **Application of rational enzyme engineering in a new route to etonogestrel and levonorgestrel: carbonyl reductase bioreduction of ethyl secodione**
Daniel F. A. R. Dourado, Andrew S. Rowan, Sergej Maciuk, Gareth Brown, Darren Gray, Jenny Spratt, Alexandra T. P. Carvalho, Dražen Pavlović, Fernando Tur, Jill Caswell, Derek J. Quinn, Thomas S. Moody and Stefan Mix
- 468 **Investigating the effect of fusion partners on the enzymatic activity and thermodynamic stability of poly(ethylene terephthalate) degrading enzymes**
Liliana Oliveira, Alex Cahill, Len Wuscher, Kerry R. Green, Victoria Bemmer and Bruce R. Lichtenstein
- 480 **Biocatalysis for industry, medicine and the circular economy: general discussion**

CONCLUDING REMARKS

- 507 **Concluding remarks: biocatalysis**
Uwe T. Bornscheuer

ADDITIONAL INFORMATION

- 516 **Poster titles**
- 521 **List of participants**

